## APXPS-2021 Virtual Workshop Agenda Brookhaven National Laboratory December 7-10, 2021

(All times are in Eastern Standard Time/UTC-05:00)

Time (Eastern Standard Time, UTC-05:00)	Tue, 12/7 Topic: Heterogeneous Catalysis	Wed, 12/8 Topic: Electrochemistry and Battery	Thu, 12/9 Topic: Materials and Interfaces	Fri, 12/10
10:00 AM	Welcome	Overview of the day	Overview of the day	
10:10 AM				
10:20 AM	Plenary 1 - Rodriguez	Invited 5 - Jeong	Invited 9 - Yamamoto	
10:30 AM	Trendry 1 Rodriguez			
10:40 AM				Technical session
10:50 AM		Invited 6 - Park	Plenary 3 - Ammann	
11:00 AM	Invited 1 - Blomberg		Fieldly 3 - Allillalli	
11:10 AM				
11:20 AM		Plenary 2 - Yano		
11:30 AM	Invited 2 - Grinter	richary 2 Tano	Invited 10 - Allen	Break
11:40 AM				2.00
11:50 AM	Contributed 1 - Garcia	Contributed 4 -	Contributed 7 - J. Wang	Contributed 10 -
12:00 PM	Martinez	Chaveanghong	contributed / 3. Wang	Goodwin
12:10 PM	Break	Break	Break	Contributed 11- Boucly
12:20 PM	Break	Dream	Dican	Contributed 11 Bodery
12:30 PM				Contributed 12 - Jones
12:40 PM	Invited 3 - Eren	Invited 7 - Yashina	Invited 11 - Bournel	
12:50 PM				Next APXPS workshop
1:00 PM				and Closeout
1:10 PM	Invited 4 - Weaver	Invited 8 - Mom	Invited 12 - Starr	
1:20 PM				
1:30 PM	Contributed 2 - Jenkins	Contributed 5 - Källquist	Contributed 8 - Gross	
1:40 PM	Co	Some some some some some some some some s	35	
1:50 PM	Contributed 3 -	Contributed 6 - Javed	Contributed 9 - Karagoz	
2:00 PM	Mosevitzky Lis	contributed o Javed	Continuated 5 Raidg02	

Pre-recorded contributed talks and poster presentations will be made available to registered workshop participants on Dec. 7-31, 2021.

Day 1: Tuesday, December 7, 2021

10:00 am – 10:10 am	Welcoming remarks – John Hill (NSLS-II Director)		
10:10 am – 10:50 am	Plenary 1 – Jose Rodriguez (Brookhaven National Laboratory)		
	"APXPS and C1 Catalysis: Fundamental Studies on the Conversion of		
	CO <sub>2</sub> and CH <sub>4</sub> "		
10:50 am – 11:20 am	Invited 1 – Sara Blomberg (Lund University)		
	"In situ APXPS applied to catalysis for renewables"		
11:20 am – 11:50 am	Invited 2 – David Grinter (Diamond Light Source)		
	"Ambient Pressure NEXAFS at VerSoX B07-B"		
11:50 am – 12:10 pm	Contributed 1 – Fernando Garcia-Martinez (Centro de Física de Materiales (CSIC - UPV/EHU))		
	"Asymmetric CO ignition on Rh stepped surfaces studied with a curved sample"		
12:10 pm – 12:30 pm	Break		
12:30 pm – 1:00 pm	Invited 3 – Baran Eren (Weizmann Institute of Science)		
	"The interaction of methanol vapor with copper surfaces"		
1:00 pm – 1:30 pm	Invited 4 – Jason Weaver (University of Florida)		
	"Methane Oxidation on IrO <sub>2</sub> (110) Thin Films"		
1:30 pm – 1:50 pm	Contributed 2 - Jessica Jenkins (Oregon State University)		
	"Reaction of 2-Propanol on SnO₂(101) and SnO₂(110) Studied using		
	Ambient-Pressure X-ray Photoelectron Spectroscopy"		
1:50 pm – 2:10 pm	Contributed 3 - Bar Mosevitzky Lis (Lehigh University)		
	"Surface-bulk dynamics of bulk mixed oxide and supported metal oxide catalysts under reaction conditions: an in situ NAP-XPS study"		

Day 2: Wednesday, December 8, 2021

10:00 am – 10:10 am	Overview of the day		
10:10 am – 10:40 am	Invited 5 – Beomgyun Jeong (Korea Basic Science Institute)		
	"Ongoing APXPS studies in Korea Basic Science Institute"		
10:40 am – 11:10 am	Invited 6 – Jeunghee Park (Korea University)		
	"Two-Dimensional Transition Metal Dichalcogenide Alloy Nanosheets to Enhance Electrocatalytic Performance"		
11:10 am – 11:50 am	Plenary 2 – Junko Yano (Lawrence Berkeley National Laboratory)		
	"Application of X-ray Techniques for Studying Artificial Photosynthetic Systems"		
11:50 am – 12:10 pm	Contributed 4 – Suwilai Chaveanghong (Institute for Molecular Science, Japan)		
	"Sulfur poisoning Pt and PtCo anode and cathode catalysts in polymer electrolyte fuel cells studied by Operando near ambient pressure hard X-ray photoelectron spectroscopy"		
12:10 pm – 12:30 pm	Break		
12:30 pm – 1:00 pm	Invited 7 – Lada Yashina (Lomonosov Moscow State University)		
	"Photoemission studies of Li-O <sub>2</sub> batteries"		
1:00 pm – 1:30 pm	Invited 8 – Rik Mom (Leiden University)		
	"Modeling of Fuel Cell and Electrolyzer processes using Electrochemical XPS and XAS data"		
1:30 pm – 1:50 pm	Contributed 5 – Ida Källquist (Uppsala University)		
	"Potentials in Li-ion batteries probed by operando APPES"		
1:50 pm – 2:10 pm	Contributed 6 – Hassan Javed (Leiden University)		
	"Platinum electrocatalyst oxidation under steady state and transient conditions examined by in situ XPS and XAS"		

Day 3: Thursday, December 9, 2021

10:00 am – 10:10 am	Overview of the day		
10:10 am – 10:40 am	Invited 9 – Susumu Yamamoto (Tohoku University)		
	"Operando observation of photo-excited carriers and molecules at solid surfaces using time-resolved XPS"		
10:40 am – 11:20 am	Plenary 3 – Markus Ammann (Paul Scherrer Institut)		
	"Surface Science in the Atmosphere"		
11:20 am – 11:50 am	Invited 10 – Heather Allen (Ohio State University)		
	"Interfacial Aqueous Organization and Electric Fields Generated from Chemical Composition: Environmental and Material Surfaces"		
11:50 am – 12:10 pm	Contributed 7 – Jiayue Wang (Massachusetts Institute of Technology)		
	"Quantifying the strain-dependent surface defect equilibria of perovskites"		
12:10 pm – 12:30 pm	Break		
12:30 pm – 1:00 pm	Invited 11 – Fabrice Bournel (Sorbonne University and Synchrotron SOLEIL)		
	"Real time NAP-XPS study of dry silicon oxidation"		
1:00 pm – 1:30 pm	Invited 12 – David Starr (Helmholtz-Zentrum Berlin)		
	"Solid-liquid interfaces studied with synchrotron-based ambient pressure X-ray photoelectron spectroscopy"		
1:30 pm – 1:50 pm	Contributed 8 – Adam Gross (University of California, Davis)		
	"Copper migration in intercalated topological insulator Cu <sub>x</sub> Bi <sub>2</sub> Se <sub>3</sub> "		
1:50 pm – 2:10 pm	Contributed 9 – Burcu Karagoz (Brookhaven National Laboratory)		
	"Surface Chemistry of NO2 and CO on a Cu2O(111) Surface"		

Day 4: Friday, December 10, 2021

10:00 am – 10:05 am	Overview of technical session		
	"Streamlining and Enabling Automated/Remotely-Controlled AP- XPS Experiments"		
	Contributions from:		
10:05 am – 10:20 am 10:20 am – 10:35 am	<ul> <li>Ignacio Villar (ALBA Synchrotron, Spain)         "Remote experiments at the CIRCE-NAPP station in ALBA"</li> <li>Patrick Zeller (BESSY, Germany)         "NAP-XPS remote operation capabilities at BESSY II"</li> </ul>		
10:35 am – 10:50 am	Luca Artiglia (Swiss Light Source/PSI, Switzerland)     "PShell software implementations to control the In Situ     Spectroscopy beamline at SLS"		
10:50 am – 11:05 am	Robert Temperton (MAX IV, Sweden)     "Enabling remote AP-XPS measurements at the HIPPIE and SPECIES beamlines at MAX IV"		
11:15 am – 11:20 am	Georg Held (Diamond Light Source, UK)  "Remote Operation at the VerSoX beamline of Diamond Light Source"		
11:20 am – 11:35 am	Slavomir Nemsak (Advanced Light Source, USA)     "Semi-automated remote APXPS experiments at the ALS"		
11:30 am – 11:50 am	Break		
11:50 am – 12:10 pm	Contributed 10 - Christopher Goodwin (Stockholm University)		
	"In situ observations of ammonia synthesis"		
12:10 pm – 12:30 pm	Contributed 11 - Anthony Boucly (Paul Scherrer Institut)		
	"Water inhibition effect and highly cationic Pd species detected by AP-XPS on Pd/Al $_2O_3$ catalysts for methane oxidation reaction"		
12:30 pm – 12:50 pm	Contributed 12 - Rosemary Jones (Lund University)		
	"AP-XPS study of the adsorption of ethanol on rutile TiO2 (110)"		
12:50 pm – 1:00 pm	Next APXPS workshop and Closeout		

#### **Pre-Recorded Contributed Talks**

	Name	Affiliation	Title
RT-01	Peter Amann	Scienta Omicron	The State of Zn under Methanol Synthesis Conditions over Zn/ZnO/Cu(211) Catalyst
RT-02	Hao Chen	Lawrence Berkeley National Laboratory	Resolving the Nature of SMSI among Au-CoO <sub>x</sub> Model Catalyst
RT-03	David Degerman	Stockholm University	Pressure hopping: Investigating CO and CO <sub>2</sub> hydrogenation on Rh in the borderlands between operando and post-mortem
RT-04	Pedro Alzaga	Oregon State University	Oxidation of amorphous metal alloy surfaces studied using ambient pressure X-ray photoelectron spectroscopy
RT-05	Heath Kersell	Oregon State University	In-situ evolution of structure and chemical state during nanoparticle exsolution from perovskite hosts by reduction in H <sub>2</sub>
RT-06	Esko Kokkonen	MAX IV Laboratory	Using Ambient Pressure XPS to study ALD in real-time
RT-07	Withdrawn	Withdrawn	Withdrawn
RT-08	Alexander Large	Diamond Light Source	Anodized aluminium as a model catalyst support material in the complete oxidation of methane
RT-09	Patrick Lömker	Stockholm University	Single crystalline Co(0001) Fischer-Tropsch observations at 550mbar (and above) using a virtual cell approach and hard X-rays
RT-10	Withdrawn	Withdrawn	Withdrawn
RT-11	Richard Oleksak	National Energy Technology Laboratory	In situ study of alloy degradation in high temperature CO <sub>2</sub>
RT-12	Christoph Rameshan	TU Wien	Tailoring of Catalyst Surfaces for Energy Conversion – In-situ Studies of Electrochemical driven Nanoparticle Exsolution

RT-13	Joachim Schnadt	Lund University	APXPS investigation of atomic layer deposition of HfO <sub>2</sub> on SiO <sub>2</sub> : evidence for a bimolecular reaction mechanism in the initial metal half-cycle
RT-14	Markus Soldemo	Stockholm University	Subsurface oxygen in oxide derived Cu catalyst for CO <sub>2</sub> reduction
RT-15	Andreas Thissen	SPECS Surface Nano Analysis GmbH	Quantification and reporting of XPS data taken under Near Ambient Pressure conditions – chances and challenges in acquisition speed, beam damage, sensitivity, reliability, reproducibility and repeatability
RT-16	Ryan Thorpe	Lehigh University	Lab-Based NAP-XPS at the Lehigh University Materials Characterization Facility
RT-17	Ryo Toyoshima	Keio University	In situ analysis of a Pt thin film H <sub>2</sub> gas sensor surface by AP-XPS
RT-18	Matthijs Van Spronsen	Diamond Light Source	Electrode-Electrolyte Interface Sensitivity in soft X-ray absorption spectroscopy via electron/ion yield
RT-19	Mykhailo Vorokhta	Charles University	Understanding the gas sensing mechanisms by NAP-XPS
RT-20	Haiko Wittkämper	FAU Erlangen- Nürnberg - Physikalische Chemie II	Spectroscopic Insights to Pt-, Pd- and Rh-Ga Alloys as Models for SCALMS Catalysts during Oxidation
RT-21	Rito Yanagi	Yale University	Operando Probing of the Energetics of Protective Coating for Solar Fuels Production
RT-22	Youngseok Yu	KBSI	Water adsorption behavior on anatase TiO <sub>2</sub> (111) utilizing Near Ambient Pressure XPS
RT-23	Xueqiang Zhang	Beijing Institute of Technology	Surface Reconstruction in In <sub>2</sub> O <sub>3</sub> /m-ZrO <sub>2</sub> Catalyzed CO <sub>2</sub> Hydrogenation

### **Pre-Recorded Poster Presentations**

	Name	Affiliation	Title
PP-01	Luca Artiglia	Paul Scherrer Institut	The In Situ Spectroscopy beamline at the Swiss light source
PP-02	Sheng Yuan Chen	National Tsing Hua University	APXPS investigation of photocatalytic nitrogen reduction reaction in Bi <sub>5</sub> O <sub>7</sub> Br <sub>0.5</sub> l <sub>0.5</sub> : the critical role played by oxygen vacancy
PP-03	Sabrina Gericke	Lund University	An in situ APXPS characterization of Al <sub>2</sub> O <sub>3</sub> supported NiMo catalyst
PP-04	Withdrawn	Withdrawn	Withdrawn
PP-05	Man Guo	Paul Scherrer Institut	Unveiling the active oxygen species in ethylene epoxidation over silver by ambient pressure X-ray photoelectron spectroscopy
PP-06	Tianhao Hu	Stony Brook University	In situ Spectroscopy Studies of Anisole Adsorption in NiMoO <sub>x</sub> Catalysts
PP-07	Nuria J. Divins	Technical University of Catalonia	Investigation of ball-milled Pd/CeO <sub>2</sub> catalysts under operando methane combustion conditions
PP-08	Moonjung Jung	GIST	Exploring chemical/electronic change of environment of platinum atom on Pt <sub>3</sub> M (M=Ti,V) alloy surface under oxidation process
PP-09	Geonhwa Kim	Pohang Accelerator Laboratory	Catalytic reactivity stud on an atomically modified glassy carbon surface
PP-10	Xiansheng Li	ETH Zurich and Paul Scherrer Institute	Structure-activity evolution of platinum species supported on ceria during Water-Gas Shift Reaction
PP-11	Hojoon Lim	Gwangju Institute of Science and Technology	Nature of the surface space charge layer on undoped SrTiO <sub>3</sub> (001)
PP-12	Bo-Hong Liu	Lawrence Berkeley National Laboratory	Ambient Pressure X-ray Photoelectron Spectroscopy Study of Room-Temperature Oxygen Adsorption on Cu(100) and Cu(111)
PP-13	Carlos Morales	Brandenburg University of Technology Cottbus— Senftenberg	Induced reduction by H <sub>2</sub> exposure at room temperature of ceria ultrathin films grown by atomic layer deposition
PP-14	Andreas Nenning	TU Wien	Voltage dependent kinetics and surface chemistry of solid oxide cell electrodes

PP-15	Philip Petzoldt	Technical University of Munich	Monitoring the Behavior of Pt Loaded TiO <sub>2</sub> (110) under Oxidizing and Reducing Conditions
PP-16	Ina Schmidt-Hanke	InProcess Instruments GmbH	Tailored Mass Spectrometry Solutions for the Gas Analysis of APXPS Systems at Different Pressure Ranges
PP-17	Minsik Seo	Gwangju Institute of Science and Technology	Investigation of surface oxidation on Pt3V alloys using ambient pressure XPS
PP-18	Stefan Van Vliet	ARCNL	Oxidation kinetics of Ru(0001) studied by NAP-XPS
PP-19	Withdrawn	Withdrawn	Withdrawn
PP-20	Chia-Hsin Wang	NSRRC	Ambient pressure/ UHV X-ray Photoelectron Spectroscopy End Stations at TPS BL43A
PP-21	Chueh Cheng Yang	National Yang Ming Chiao Tung University	Investigation of Redox Reaction of Platinum during Electrochemical Catalysis Reaction by Ambient Pressure XPS
PP-22	Youngseok Yu	KBSI	Surface chemical states of carbon-steel utilizing near ambient pressure XPS